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# On the Essential Role of Kinetic Theory in Numerical Methods for Fluid-Dynamic Equations

Taku Ohwada<sup>a</sup> and Pietro Asinari<sup>b</sup>

<sup>a</sup> *Department of Aeronautics and Astronautics, Graduate School of Engineering,  
Kyoto University, Kyoto 606-8501, JAPAN*

<sup>b</sup> *Dipartimento di Energetica, Politecnico di Torino, Torino 10129, ITALY*

**Abstract.** The essential role of kinetic theory in the numerical methods for the Navier-Stokes equations (compressible and incompressible) is discussed. The easy theory of characteristics for kinetic equations brings about drastic simplification of approximate Riemann solver employed in various shock-capturing schemes. The lattice Boltzmann method is shown to essentially solve an artificial compressibility PDE system. The asymptotic behavior of solution of kinetic equations for small mean free path does not play the essential role in these kinetic numerical methods.

**Keywords:** Kinetic Scheme, Gas Kinetic, Lattice Boltzmann, Euler Equations, Navier-Stokes Equations

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## INTRODUCTION

Kinetic theory of gases provides the theoretical basis of fluid dynamics. In recent years, it has been making remarkable contribution to the development of numerical methods for fluid-dynamic equations. Indeed, the employment of kinetic equation drastically simplifies the theory of characteristics in the approximate Riemann solver and some computational advantages of the kinetic approach over the conventional continuum-based one have been reported [e.g. the adaptability of the Lattice Boltzmann Method (LBM) to large parallel computation]. However, it is not too much to say that the indirect formulation of kinetic approach, i.e. the employment of distribution function of gas molecules and its asymptotic behavior for small mean free path, becomes a major obstacle to the prevalence in the engineering community at large.

It is often said nowadays that CFD is in quite a matured state. The settlement of a new formulation in this situation requires its very clear outcome. The present article focuses on the outcome of kinetic formulation in the numerical methods for the compressible Navier-Stokes equations (CNSE) and the incompressible NS equations (INSE). The first part of the present article is for CNSE and is based on the results in [1]-[4]. The second part is about the authors' recent theoretical and numerical study for LBM [5] and new results are included there.

## CASE OF COMPRESSIBLE FLOWS

We start the review of kinetic schemes with a brief explanation of Pullin's Equilibrium Flux Method (EFM) for the compressible Euler equations (CEE) [6], which is one of the origins of kinetic schemes. Its formulation is strongly affected by DSMC, where the coordinates of particles in phase space are updated in two steps, i.e. the free flow step corresponding to the solution for the collisionless Boltzmann equation and the collision step corresponding to that for the spatially homogeneous Boltzmann equation. Similar to DSMC, the computational domain of EFM is divided into cells (finite volume method) and the numerical flux is computed from the solution of the collisionless Boltzmann equation for an initial equilibrium state. The new equilibrium state, which is employed as the initial data for the computation of next time step, is created from the updated macroscopic variables, which corresponds to the collision step for the time step much larger than the mean free time. Mandel and Deshpande [7] derived the same DSMC-based scheme and called it Kinetic Flux Vector Splitting (KFVS) scheme. Hereafter, we will use "KFVS"

instead of “DSMC-based” according to the convention. Chou and Baganoff [8] extended KFVS to the case of CNSE by introducing Chapman-Enskog distribution function, which yields the viscous stress and heat flow of CNSE. The first successful kinetic scheme for CNSE, called Gas Kinetic BGK (GKB) scheme, was developed by Xu [9], who employed the solution of the BGK equation to compute the numerical flux; the effect of molecular collision is taken into account explicitly there, which is in contrast to KFVS schemes. KFVS and GKB are sophisticated by the implementation of the reconstruction technique in CFD, such as MUSCL, and are shock-capturing; a shock wave is well captured within a few mesh points (cells) without spurious oscillations. While GKB is able to produce a fine viscous boundary-layer profile with a reasonable resolution, e.g. ten cells in the layer, the result of KFVS is very poor under the same resolution. Despite its high performance, the mechanism of GKB was not transparent. Ohwada proposed a method for the construction of kinetic equation that is directly related to the target macroscopic equation (or system) together with some numerical examples in [1]. The mechanism of Xu’s GKB scheme was finally solved by the analysis of [2], where the relation to the Lax-Wendroff scheme is revealed, and that of [3], where the role of kinetic reconstruction of fluid-dynamic variables is clarified. The key extracted from GKB is very useful for the construction of simple but capable kinetic schemes for CNSE, which is demonstrated in [4]. Subsequent to the above overview of development history of kinetic schemes, we will discuss the essential role of kinetic theory in the case of compressible flow solver.

## Kinetic Scheme for Compressible Euler Equations

We will clarify the essential role of kinetic theory by demonstrating the construction of a capable kinetic scheme. In this subsection, we will derive a kinetic scheme for 1D CEE:

$$\frac{\partial \vec{h}}{\partial t} + \frac{\partial \vec{\Phi}}{\partial x} = 0, \quad (1)$$

where  $x$  and  $t$  are the space coordinate and the time, respectively, the elements of the vector  $\vec{h}$  are the conservative variables, and those of the vector  $\vec{\Phi}$  are the corresponding flux functions. We summarize the minimum kinetic gadgets. In order to avoid unessential complexities, we consider the case of a monatomic gas. We introduce the distribution function  $f(x, t, \xi_i)$ , where  $\xi_i$  is the molecular velocity. The extension to the case of polyatomic gas is done straightforwardly according to the rotational degree of freedom, e.g.  $f(x, t, \xi_i, \eta_1, \eta_2)$  for a diatomic molecular gas, and the extension to the case of multi-dimensional flows is an easy exercise of the divergence theorem. The macroscopic variables are given by the moments of the distribution function:

$$\vec{h} = \int \vec{\varphi} f d\vec{\xi}, \quad (2)$$

where the elements of the vector  $\vec{\varphi}$  are the summational invariants,  $d\vec{\xi} = d\xi_1 d\xi_2 d\xi_3$ , and the domain of integration with respect to  $\xi_i$  is the whole velocity space. Next, we introduce the equilibrium distribution function  $f_0$ , which has the following properties.

- (i) The equilibrium distribution function depends on  $x$  and  $t$  only through  $\vec{h}$ , i.e.  $f_0 = f_0(\vec{h}(x, t), \xi_i)$ .
- (ii) The conservative variables  $\vec{h}$  and the flux functions  $\vec{\Phi}$  of CEE are given by the following moments of  $f_0$ :

$$\vec{h} = \int \vec{\varphi} f_0 d\vec{\xi}, \quad (3)$$

$$\vec{\Phi} = \int \xi_1 \vec{\varphi} f_0 d\vec{\xi}, \quad (4)$$

where  $\xi_1$  is the component of molecular velocity in the direction of  $x$ . We emphasize that the above kinetic gadgets suffice for the construction of capable kinetic schemes. The Maxwellian is the classic equilibrium distribution function but other equilibrium distribution functions are available as will be mentioned later.

Suppose a distribution function in the form of the equilibrium distribution function, i.e.  $f(x, t, \xi_i) = f_0(\vec{h}(x, t), \xi_i)$ , and let its macroscopic parameters  $\vec{h}$  satisfy CEE (1). It is easy to verify that such a distribution function satisfies the following kinetic equation:

$$\frac{\partial f}{\partial t} + \xi_1 \frac{\partial f}{\partial x} = \mathcal{Q}[f], \quad (5a)$$

$$\mathcal{Q}[f] = -\frac{\partial f_0}{\partial \vec{h}} \cdot \frac{\partial \vec{\Phi}}{\partial x} + \xi_1 \frac{\partial f_0}{\partial x}, \quad (5b)$$

where  $Q[f]$  is computed from  $f$  by using Eqs.(2) and (5b). Assuming the uniqueness of solution of Eq.(5), we can get the solution of Eq.(1) via Eq.(5). The numerical scheme is constructed by making use of Eq.(5) as the railroad of CEE. Incidentally, the other equations, such as

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} = -\frac{\partial f_0}{\partial \vec{h}} \cdot \frac{\partial \vec{\Phi}}{\partial x} + \frac{\partial f_0}{\partial x}, \quad (6a)$$

$$\frac{\partial f}{\partial t} - \frac{\partial^2 f}{\partial x^2} = -\left( \frac{\partial f_0}{\partial \vec{h}} \cdot \frac{\partial \vec{\Phi}}{\partial x} + \frac{\partial^2 f_0}{\partial x^2} \right), \quad (6b)$$

can be considered as the candidates of the railroad. The reason why Eqs.(6a) and (6b) are excluded will be seen later.

The finite volume formula for Eq.(1) is derived from Eq.(5a) by multiplying both sides by  $\vec{\varphi}$  and integrating the result over the whole velocity space, the space interval  $x_{i-1/2} < x < x_{i+1/2}$ , and the time interval  $0 < t < \Delta t$ :

$$\vec{H}_i(\Delta t) = \vec{H}_i(0) - \frac{\vec{F}_{i+1/2} - \vec{F}_{i-1/2}}{x_{i+1/2} - x_{i-1/2}}, \quad (7a)$$

$$\vec{H}_i(t) \equiv \frac{1}{x_{i+1/2} - x_{i-1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \vec{h}(x, t) dx, \quad (7b)$$

$$\vec{F}_{i+1/2} \equiv \int_0^{\Delta t} \int \xi_1 \vec{\varphi} f(x_{i+1/2}, t, \xi_i) d\xi dt. \quad (7c)$$

The right hand side of Eq.(5a) vanishes after the integration with respect to the molecular velocity because of Eqs.(3) and (4). The numerical flux is given by the moment of solution of Eq.(5). Incidentally, in the case of Eqs.(6a) and (6b), the numerical flux is expressed as the time integration of the flux function  $\vec{\Phi}$  and no trace of kinetic formulation is left in the resulting formula.

Similar to the case of the Boltzmann equation, the solution of Eq.(5a) is formally expressed in the integral form along the characteristics. For the numerical flux with second order accuracy in time, the approximation

$$f(x_{i+1/2}, t, \xi_i) = f_0(x_{i+1/2}, 0, \xi_i) - t \xi_1 \frac{\partial f_0}{\partial x}(x_{i+1/2}, 0, \xi_i) + t Q[f](x_{i+1/2}, 0, \xi_i), \quad (8)$$

suffices, where the initial data is given in the form of the equilibrium distribution function, i.e.  $f(t=0) = f_0$ . The formula (7a) gives the cell-averaged value of  $\vec{h}$ . In order to compute the numerical flux, the distributions of the primitive variables, such as  $\rho$ ,  $u_i$ , and  $T$ , must be reconstructed from the cell-averaged values. If the reconstructed distribution is the piecewise linear one made by simply connecting the cell-center values, then the distribution is smooth around cell interfaces ( $x = x_{i+1/2}$ ), and the finite volume method becomes the Lax-Wendroff-type; no trace of kinetic formulation is left there. This is the natural consequence from the consistency of the scheme. The kinetic formulation is meaningful only in the case of discontinuous reconstruction, such as MUSCL. In this case, there are two limiting values for  $x = x_{i+1/2} \pm 0$  at the cell interface  $x = x_{i+1/2}$ . The easy theory of characteristics for the kinetic equation provides the clear principle of the choice; the value for  $x = x_{i+1/2} - 0$  is chosen for  $\xi_1 > 0$  and vice versa. Therefore,  $f$  in Eq. (7c) is divided into two parts. The functional form of the equilibrium distribution function should be such that the integration with respect to the molecular velocity for  $\xi_1 > 0$  and that for  $\xi_1 < 0$  can be done analytically in advance. In the case of the classic Maxwellian, the error function appears in the formula of numerical flux. In the case of Perthame's artificial equilibrium distribution function [10], which has compact support, the formula is expressed only by using fundamental arithmetic and the resulting scheme is more efficient.

## Extension to NS Equations

The employment of Chapman-Enskog distribution function seems to be a natural choice in the extension to the case of CNSE as found in [1,8,9]. On the other hand, the trace of kinetic formulation disappears in the case of continuous reconstruction of fluid-dynamic variables. We will reexamine this seemingly reasonable extension in connection with the reconstruction.

The kinetic railroad for CNSE is constructed in a similar way to the case of CEE. The distribution function is composed of the equilibrium distribution function and its correction, i.e.  $f = f_0 + f_c$ . Since  $f_0$  yields  $\vec{h}$  and  $\vec{\Phi}$ , the correction  $f_c$  must be orthogonal to  $\vec{\varphi}$ , yielding the dissipative flux of CNSE. In addition, we consider the case where the ratio of  $f_c$  to  $f_0$ , which is of the order of the inverse Reynolds number (or the Knudsen number), is very

small and the magnitude of dimensionless time step employed in the computation is larger than or the same order of the ratio. Under this usual situation, we can employ without loss of high accuracy

$$f(x_{i+1/2}, t, \xi_i) = f_0(x_{i+1/2}, 0, \xi_i) + f_c(x_{i+1/2}, 0, \xi_i) - t\xi_i \frac{\partial f_0}{\partial x}(x_{i+1/2}, 0, \xi_i) + tQ[f](x_{i+1/2}, 0, \xi_i), \quad (9)$$

as the extension of Eq.(8) to the case of CNSE. Recall the fact that the introduction of discontinuous reconstruction is for shock-capturing. The numerical dissipation produces by the discontinuities suppresses spurious oscillations around shocks and contact surfaces. Since the numerical dissipation produced by the discontinuous reconstruction of  $f_0$  is much larger than that of  $f_c$ , we need not deliberately apply discontinuous approximation to  $f_c$ . In this way, no trace of kinetic formulation is left in the dissipative numerical flux, which is simply approximated by usual finite difference formulas. In other words, the Chapman-Enskog distribution function and its artificial substitute are meaningless. This finding based on the numerical consideration (Egg of Columbus!) drastically simplifies the theory of kinetic scheme for CNSE. Incidentally, a kinetic scheme for the Burnett equations is developed by using this key together with a high order time integration formula of kinetic equation in [11].

Finally, we mention a side effect of discontinuous reconstruction and the cure. The numerical dissipation of discontinuous reconstruction is usually very small in a smooth region. However, it is not negligibly smaller than the physical dissipation in the case of boundary-layer without an excessively high resolution. This is in contrast to the Lax-Wendroff-type scheme, which yields a fine boundary layer profile under a reasonable resolution. It is natural to consider the hybridization of Lax-Wendroff scheme and the scheme for discontinuous reconstruction. However, it is not easy to blend these schemes of different types. In GKB scheme, another kinetic reconstruction, which is less dissipative than the usual discontinuous one and is more dissipative than the continuous one, is employed in the approximation of the gain term of BGK equation. The scheme employing only this less dissipative kinetic reconstruction works quite well; it yields a fine result in Blasius flow problem and blast-wave test case but produces small spurious oscillations around the tail of the expansion wave in Sod test case [3]. The BGK solution in GKB scheme plays the role of blender of two schemes for the discontinuous reconstruction and the less dissipative kinetic reconstruction. A simple and capable hybrid kinetic scheme for CNSE is developed in [4] by making use of this key. The outcome of kinetic formulation lies only in the reconstruction, which is a summary of this section.

## CASE OF INCOMPRESSIBLE FLOWS

### Theory of LBM

LBM is now recognized as a promising numerical method for fluid-dynamic equations, such as the incompressible NS equations (INSE), which is its main target equation system. The application of LBM is diversifying, such as the compressible flows, micro flows, multi-phase flows, blood flows and so on. However, it is beyond the scope of the present article to cover all the contributions of LBM. We focus on its fundamental nature here and refer the reader to Ref.[12] for its recent coverage of various applications.

The discrete velocity model of isothermal BGK equation with a constant collision frequency is widely employed as the basis of LBM. Because of the limited space, we will explain only the essence of LBM; we refer the reader to [13-15] for the technical details. Let  $V_i$  ( $i = 1, 2$ ) be the component of the dimensionless molecular velocity in the  $x_i$  direction. The following discussion is for its D2Q9 model, which deals with 9 velocities in 2D velocity space, i.e.  $(V_1, V_2) = (0, 0), (1, 0), (1, 1), (0, 1), (-1, 1), (-1, 0), (-1, -1), (0, -1), (1, -1)$ . The coordinates of spatial lattice points are given by  $(\hat{x}_1, \hat{x}_2) = (l, m)$ , where  $l$  and  $m$  are integers. The “molecule” at the spatial lattice point  $(\hat{x}_1^P, \hat{x}_2^P)$  moves to  $(\hat{x}_1^P + V_1, \hat{x}_2^P + V_2)$ , which is one of the lattice points in the stencil for  $(\hat{x}_1^P, \hat{x}_2^P)$ , during the unit time step. The dimensionless density  $\rho$  and flow velocity  $u_i$  are computed from the distribution function  $\hat{f}(\hat{t}, \hat{x}_i, V_i)$  as  $\rho = \langle \hat{f} \rangle$  and  $u_i = \langle V_i \hat{f} \rangle$ , where  $\langle \dots \rangle$  means the sum over all the velocities. The updating rule of distribution function in LBM is nothing more than the forward Euler time integration of the dimensionless discrete velocity BGK equation along its characteristics:

$$\hat{f}(\hat{x}_i, \hat{t} + 1, V_i) = \hat{f}(\hat{x}_i - V_i, \hat{t}, V_i) + \lambda[\hat{f}_e - \hat{f}](\hat{x}_i - V_i, \hat{t}, V_i), \quad (10)$$

where  $\hat{f}_e$  is the discrete equilibrium distribution function, the each element of which is characterized only by the macroscopic variables, and  $\lambda$  is a positive constant of the order of unity. Owing to the arrangement of velocities and the lattice points, the interpolation is avoided in Eq. (10). It is seen from the analogy to the integral form of the continuous BGK equation that the units of speed, time, and length in the above updating rule correspond to the thermal speed, the mean free time, and the mean free path, respectively. Obviously, these units are not appropriate

for the description of incompressible continuum flow field. Let the characteristic length and the characteristic speed of the flow under consideration be  $L$  and  $U$ , respectively, and let the characteristic time of the flow be of the order of  $L/U$ . We denote the mean free path and the thermal speed by  $l_c$  and  $c$ , respectively, and introduce the new dimensionless coordinates  $x_i$  and  $t$  defined by  $x_i = (l_c/L)\hat{x}_i$  and  $t = (l_c U/Lc)\hat{t}$ , respectively. The continuum limit implies  $l_c \ll L$  and the incompressible limit means  $U \ll c$ . Defining the small parameter  $\varepsilon$  as  $\varepsilon = l_c/L$  (the Knudsen number), we have  $x_i = \varepsilon \hat{x}_i$ . Further, assuming  $U/c = \varepsilon$ , which is the key of the incompressible continuum (diffusive) limit [16,17], we have  $t = \varepsilon^2 \hat{t}$ . Then, Eq.(10) is rewritten as

$$f(x_i, t + \varepsilon^2, V_i) = f(x_i - \varepsilon V_i, t, V_i) + \lambda[f_e - f](x_i - \varepsilon V_i, t, V_i), \quad (11)$$

where  $f(x_i, t, V_i) = \hat{f}(\hat{x}_i, \hat{t}, V_i)$  and  $f_e(x_i, t, V_i) = \hat{f}_e(\hat{x}_i, \hat{t}, V_i)$ . It is easily found from Eq.(11) that the lattice spacing is  $\varepsilon$ , i.e. Mach number or Knudsen number, which is the key of LBM. The asymptotic analysis of the updating rule (11) for small  $\varepsilon$  is carried out in [5] according to the recipe of [18], where the asymptotic behavior of MRT-LBM [19] is studied. From the analysis the following sequence of PDE systems are derived:

$$\frac{\partial u_i^{(1)}}{\partial x_i} = 0, \quad (12a)$$

$$\frac{\partial u_i^{(1)}}{\partial t} + u_j^{(1)} \frac{\partial u_i^{(1)}}{\partial x_j} + \frac{1}{3} \frac{\partial \rho^{(2)}}{\partial x_i} = \frac{1}{3} \left( \frac{1}{\lambda} - \frac{1}{2} \right) \frac{\partial^2 u_i^{(1)}}{\partial x_k^2}, \quad (12b)$$

$$\frac{\partial u_i^{(2)}}{\partial x_i} = 0, \quad (13a)$$

$$\frac{\partial u_i^{(2)}}{\partial t} + u_j^{(1)} \frac{\partial u_i^{(2)}}{\partial x_j} + u_j^{(2)} \frac{\partial u_i^{(1)}}{\partial x_j} + \frac{1}{3} \frac{\partial \rho^{(3)}}{\partial x_i} = \frac{1}{3} \left( \frac{1}{\lambda} - \frac{1}{2} \right) \frac{\partial^2 u_i^{(2)}}{\partial x_k^2}, \quad (13b)$$

where  $\rho$  and  $u_i$  are expanded as  $\rho = 1 + \varepsilon^2 \rho^{(2)} + \varepsilon^3 \rho^{(3)} + \dots$  and  $u_i = \varepsilon u_i^{(1)} + \varepsilon^2 u_i^{(2)} + \varepsilon^3 u_i^{(3)} + \dots$  (the original expansion of  $\rho$  involves the term  $\varepsilon \rho^{(1)}$  but  $\partial \rho^{(1)} / \partial x_i = 0$  is derived from the analysis and  $\rho^{(1)} = 0$  follows from the conservation of total mass). The leading equation system is INSE and a homogeneous Oseen-type equation system, which allows the null solution, follows. The third equation system, which is for  $(\rho^{(4)}, u_i^{(3)})$ , is inhomogeneous Oseen-type, and therefore, it yields the principal error for the solution of INSE. The lattice spacing and the time step correspond to  $\varepsilon$  and  $\varepsilon^2$ , respectively, and therefore, the accuracy of LBM is regarded as second order in space and first order in time. Incidentally, the third equation system involves a fake rarefaction effect term. A small stencil, such as D2Q9, cannot yield correct constitution law beyond NS; needless to say, the increase of the stencil spoils the advantage of LBM. Some misleading claims concerning the capability of LBM with a small stencil as a solver for fluid-dynamic equations beyond NS are found elsewhere.

## Artificial Compressibility Method Revisited

One of the main characteristics of LBM is that the pressure field of the incompressible fluids, i.e.  $\rho^{(2)}/3$  in Eq.(12b), is obtained evolutionarily, which reminds us of Chorin's artificial compressibility method (ACM) [20]. Chorin's idea is to replace the solenoidal condition by an artificial continuity equation with the pressure time derivative. ACM deals with the following artificial compressibility system (ACS):

$$b \frac{\partial P}{\partial t} + \frac{\partial u_i}{\partial x_i} = 0, \quad (14a)$$

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial P}{\partial x_i} = \nu \frac{\partial^2 u_i}{\partial x_k^2}, \quad (14b)$$

where  $b$  is a positive constant and  $\nu$  corresponds to the inverse Reynolds number. Incidentally, the convergence to the solution of INSE in the limit of  $b \rightarrow 0$  is studied in [21,22]. The formal asymptotic analysis using the (Mach number) expansion,  $u_i = u_i^{(0)} + b^{1/2} u_i^{(1)} + b u_i^{(2)} + \dots$  and  $P = P^{(0)} + b^{1/2} P^{(1)} + b P^{(2)} + \dots$ , derives INSE for  $(u_i^{(0)}, P^{(0)})$ , the homogeneous Oseen-type equations for  $(u_i^{(2m-1)}, P^{(2m-1)})$ , and inhomogeneous Oseen-type equation systems for  $(u_i^{(2m)}, P^{(2m)})$  ( $m = 1, 2, 3, \dots$ ). Next, we will explain the numerical realization of the above

asymptotic passage. Let us consider the case where the employed finite difference scheme is first order accurate in time and second order accurate in space and let the mesh spacing and the time step be  $\Delta x \sim b^{1/2}$  and  $\Delta t \sim b$ , respectively; the time step  $\Delta t \sim (\Delta x)^2$  satisfies the acoustic CFL condition since the speed of acoustic wave derived from Eq.(14) is  $O(1/\Delta x) \sim O(b^{-1/2})$ . The asymptotic analysis for the finite difference scheme shows that the equation systems for  $(u_i^{(0)}, P^{(0)})$  and  $(u_i^{(1)}, P^{(1)})$  are not altered and the discretization error appears as the additional source terms in the equation system for  $(u_i^{(2)}, P^{(2)})$ . Thus, the finite difference scheme can be regarded as an asymptotic numerical method for INSE and its accuracy is second order in space and first order in time, which is the same as in the case of LBM. Indeed, ACS is recovered approximately by summing up the PDE systems obtained by the asymptotic analysis of the LBM. In other words, LBM essentially solves the ACS with the mesh-dependent coefficient of pressure time derivative. Incidentally, there is a direct relation between ACM and the Lattice Kinetic Scheme [23], which is a variant of LBM. The updating rule of LKS corresponds to Eq.(10) with  $\lambda = 1$ . The values of distribution function are given by those of the equilibrium distribution functions at the different lattice points in the stencil; the equilibrium distribution function of LKS is slightly modified for the tunable Reynolds number but it is characterized only by the macroscopic variables as before. It is easily found from this fact that no trace of kinetic formulation is left in the updating rule of the macroscopic data. Indeed, LKS is a kind of finite difference scheme for ACS as shown in [5], where the improvement of stability and the reduction of stencil are proposed on the basis of this interpretation.

## Extension of Artificial Compressibility Method

In the previous subsection, we discussed the relation between LBM and ACM. While LBM is kinetic based and it yields the solution of INSE in the limit of  $\text{Kn} \sim \text{Ma} \sim \varepsilon \rightarrow 0$ , only the limit of  $\text{Ma} \sim \varepsilon \rightarrow 0$  is considered in the case of ACM (Kn, Ma, and  $\varepsilon$  stand for the Knudsen number, the Mach number, and the mesh spacing, respectively). Since ACM is a macroscopic finite difference method, its improvement seems to be more tractable than that of LBM. In this subsection, we introduce a method for the improvement of accuracy of ACM.

Since the leading error of ACS for INSE solution is proportional to  $b$ , it can be eliminated by computing the appropriate linear combination of two solutions for different values of  $b$ ; the leading error becomes  $O(b^2)$  after the cancellation. Let us write  $b$  as  $\beta \varepsilon^2$ ; the different value of  $b$  under the same resolution means the different value of  $\beta$ . For the realization of the above scenario in the numerical computation, i.e. the numerical solution with forth order accuracy in  $\varepsilon$ , the accuracy of spatial discretization must be at least forth order and that of time integration must be at least second order ( $\Delta t \sim \varepsilon^2$ ), which can be realized by employing the conventional numerical techniques, such as five point finite difference formula and second order Runge-Kutta method. However, there is an intrinsic difficulty in this approach, which will be explained below.

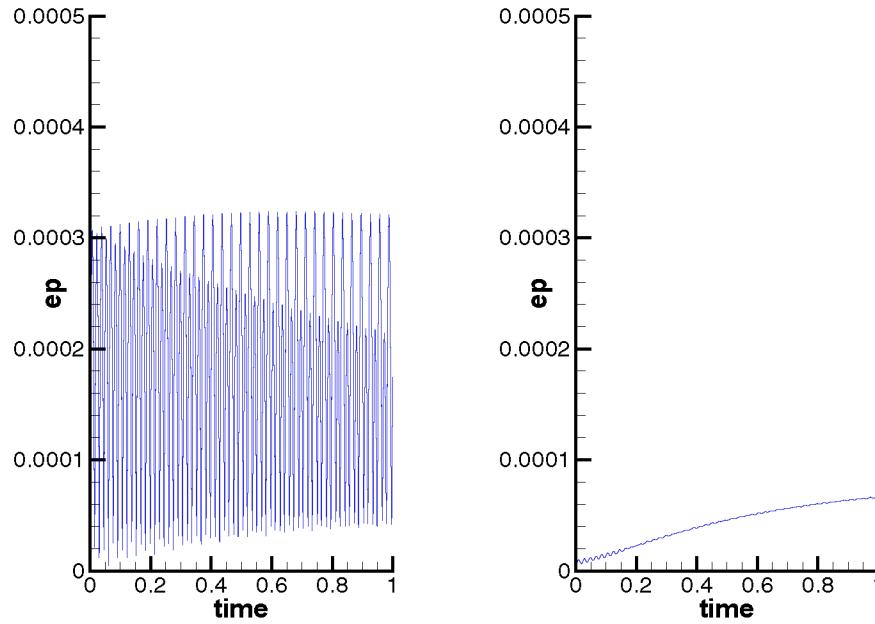
The derivation of INSE and Oseen-type equations from ACS (14) requires the assumption of slow solution, the characteristic time of which is of the order of unity. ACS also involves the fast solution, i.e. the acoustic wave. Suppose that the computation of ACS starts from the initial data compatible with INSE, i.e. a solenoidal velocity field and a solution of corresponding Poisson equation. Then, the pressure time derivative of ACS solution is zero at  $t = 0$ , while that of INSE solution is not. This difference acts as an initial impact and the fast solution is excited. It is estimated under the assumption of slow spatial variation [the wavelength is  $O(1)$ ] that the characteristic time of acoustic wave is  $O(\varepsilon)$  and the magnitude is  $O(\varepsilon^2)$  for the flow velocity and  $O(\varepsilon)$  for the pressure. Therefore, the suppression of acoustic wave is critical for the abovementioned scenario. One of the methods is the employment of the high order slow solution  $h = h^{(0)} + b h^{(2)} + \dots$  ( $h = u_i, P$ ) as the initial data, which is in the same spirit as Kreiss's bounded derivative method [24]. The computation of high order slow solution requires high order time derivatives of solution of INSE at  $t = 0$ , which is reduced to the solution of elliptic equations. Fig.1 shows the time history of  $L^1$ -error for  $P$  ( $\nu = 0.002, \beta = 6, \varepsilon = 1/40$ ) in the problem of Taylor-Green vortex in a periodic square domain of the unit area. By introducing the high order slow solution  $(u_i^{(0)} + b u_i^{(2)}, P^{(0)} + b P^{(2)})$  as the initial data, the amplitude of the excited acoustic wave is remarkably reduced, although it is not sufficient for the realization of fourth order accuracy. The preparation of special initial data is, however, costly in practical engineering problems, although it is academically interesting. Another approach is the introduction of a simple damping mechanism:

$$b \left[ \frac{\partial P}{\partial t} + \gamma P \right] + \frac{\partial u_i}{\partial x_i} = 0, \quad (15)$$

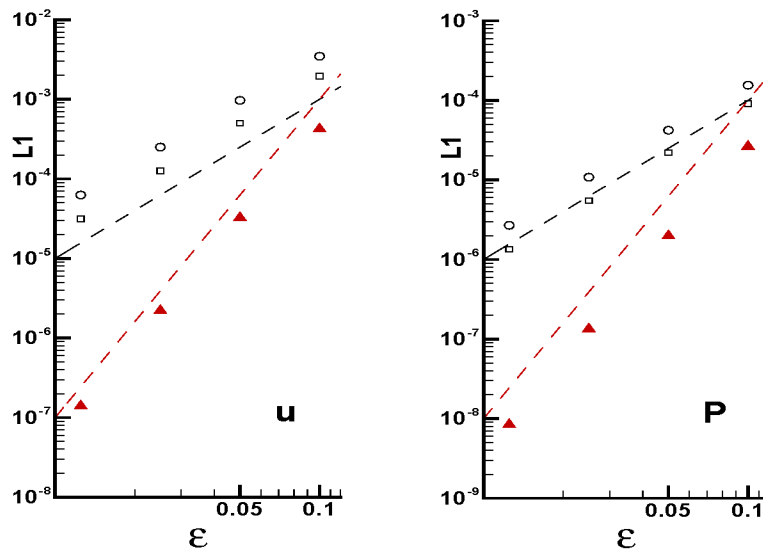
where  $\gamma$  is a positive constant of the order of unity. Without introducing the special initial data, the oscillations caused by the imperfect initial data is weakened as time passes and the solution of ACS finally reaches the slowly



varying trajectory. Fig.2 shows the convergence rates of solution of ACS after the extinction of acoustic oscillations;  $\nu = 0.002, \gamma = 10, t = 1$ , and the initial data is for  $(u_i^{(0)}, P^{(0)})$ . While the result for  $\beta = 3$  (square) and that for  $\beta = 6$  (circle) show the second order convergence rate in  $\varepsilon$ , their linear combination  $2h(\beta = 3) - h(\beta = 6)$  (triangle) clearly shows the fourth order convergence rate, although the linearity of the leading error in  $\beta$  after the extinction of acoustic wave has not yet been justified mathematically to the authors' best of knowledge.



**FIGURE1.** The time history of  $L^1$  error for  $P$ . Left: the case of the initial data  $(u_i^{(0)}, P^{(0)})$ ; Right: the case of initial data  $(u_i^{(0)} + bu_i^{(2)}, P^{(0)} + bP^{(2)})$ .



**FIGURE2.**  $L^1$  error vs.  $\varepsilon$ . The dashed lines indicate the second and fourth order convergence rate.

## CONCLUDING REMARKS

The essential role of kinetic theory in the numerical methods for CNSE and INSE is discussed. The outcome of kinetic formulation has been found only in the discontinuous reconstruction for shock capturing and its cure. The elementary kinetic theory brings about a drastic simplification of approximate Riemann solver and capable schemes are derived as the extension of the well-known Lax-Wendroff scheme without detouring via the Boltzmann equation or its asymptotic analyses. This simple kinetic formulation enables the education of high-resolution shock-capturing schemes for students without the introduction of “black box”. LBM essentially solves ACS and the superiority of the extended ACM over LBM for the accuracy is clearly demonstrated. However, this does not deny the possibility of improvement of performance by kinetic approach. We hope that the present study could stimulate further studies of LBM from this point of view. The application of the extended ACM in various engineering problems is left as a future subject. The present article also brings up a mathematical problem, i.e. the asymptotic behavior of solution of ACS with a damping term, where not only the convergence to the INSE solution but also the behavior of the deviation is the subject of consideration.

## REFERENCES

1. T. Ohwada, “Boltzmann schemes for the compressible Navier-Stokes equations”, in *Rarefied Gas Dynamics* AIP Conference Proceedings 585, edited by T.J. Bartel and M. Gallis, American Institute of Physics, pp.321-328 (2001).
2. T. Ohwada, “On the construction of kinetic schemes”, *J. Comput. Phys.* **177**, 156-175 (2002).
3. T. Ohwada and S. Kobayashi, “Management of discontinuous reconstruction in kinetic schemes”, *J. Comput. Phys.* **197**, 116-138 (2004).
4. T. Ohwada and S. Fukata, “Simple derivation of high-resolution schemes for compressible flows by kinetic approach”, *J. Comput. Phys.* **211**, 424-447 (2006).
5. P. Asinari and T. Ohwada, “Connection between kinetic methods for fluid-dynamic equations and macroscopic finite-difference schemes”, *Comput. Math. Appl.* (2008) (in Press).
6. D. I. Pullin, “Direct simulation methods for compressible inviscid ideal gas flow”, *J. Comput. Phys.* **34**, 231-244 (1980).
7. J.C. Mandal and S.M. Deshpande, “Kinetic Flux Vector Splitting for Euler Equations”, *Comput. Fluids* **23**, 447-478 (1994).
8. S.Y. Chou and D. Baganoff, “Kinetic flux-vector splitting for the Navier-Stokes equations”, *J. Comput. Phys.* **130**, 217-230 (1997).
9. K. Xu, “A gas-kinetic BGK scheme for the Navier-Stokes equations and its connection with artificial dissipation and Godunov method”, *J. Comput. Phys.* **171**, 289-335 (2001).
10. B. Perthame, “Second-order Boltzmann schemes for the compressible Euler equations in one and two space dimensions”, *SIAM J. Numer. Anal.* **29**, 1-19 (1992).
11. T. Ohwada and K. Xu, “The kinetic scheme for the full-Burnett equations”, *J. Comput. Phys.* **201**, 315-332 (2004).
12. S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond*, Oxford University Press, (2001).
13. Y. Qian, D. d’Humières, and P. Lallemand, “Lattice BGK models for Navier-Stokes equation”, *Europhys. Lett.* **17**, 479-484 (1992).
14. T. Abe, “Derivation of the lattice Boltzmann method by means of the discrete ordinate method for the Boltzmann equation”, *J. Comput. Phys.* **131**, 241-246 (1997).
15. S. Chen and G. D. Doolen, “Lattice Boltzmann method for fluid flows”, *Ann. Rev. Fluid Mech.* **30**, 329-364 (1998).
16. Y. Sone, “Asymptotic theory of flow of rarefied gas over a smooth boundary II”, in *Rarefied Gas Dynamics*, edited by D. Dini, Editrice Tecnico Scientifica, Pisa, pp.737-749 (1971).
17. C. Bardos, F. Golse, and C.D. Levermore, “Fluid dynamic limits of kinetic equations I. Formal derivations”, *J. Stat. Phys.* **63**, 323-344 (1991).
18. M. Junk, A. Klar, and L.-S. Luo, “Asymptotic analysis of the lattice Boltzmann equation”, *J. Comput. Phys.* **210**, 676-704 (2005).
19. D. d’Humières, “Generalized lattice-Boltzmann equations”, in *Rarefied Gas Dynamics: Theory and Applications*, Progress in Astronautics and Aeronautics **159**, edited by D. Shizgal and D.P. Weaver, AIAA, pp. 450-458 (1992).
20. A.J. Chorin, “A numerical method for solving incompressible viscous flow problems”, *J. Comput. Phys.* **2**, 12-26 (1967).
21. R. Témam, “Sur l’approximation de la solution des équations de Navier Stokes par la méthode des pas fractionnaires. I”, *Arch. Ration. Mech. Anal.* **32**, 135-153 (1969).
22. S. Klainerman and A. Majda, “Singular limits of quasilinear Hyperbolic Systems with large parameters and incompressible limit of compressible fluids”, *Comm. Pure Appl. Math.* **34**, 481-524 (1981).
23. T. Inamuro, “A lattice kinetic scheme for incompressible viscous thermal flows with heat transfer”, *Phil. Trans. Royal Soc. A* **360**, 477-484 (2001).
24. G. Browning, A. Kasahara, and H.-O. Kreiss, “Initialization of the primitive equations by the bounded derivative method”, *J. Atmos. Sci.*, **37**, 1424-1436 (1980).